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Vibrational transition probabilities and r-centroids of the B-X band system of SiN

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An information about the variation in electronic transition moment can be obtained from the knowledge of Franck-Condon factors, *r*-centroids and the intensity distribution in a band system. The $B^2\Sigma^+ \rightarrow X^2\Sigma^+$ band system of

Table 1. Morse Franck-Condon factors and *r*-centroids for the *B–X* band system of SiN

	*(*a*)	0·9922	0·0043	0·0008	0·0011	0·0000
	**(*b*)	1·595	—	—	—	—
0	+(*c*)	1·600	—	—	—	—
	++(*d*)	4116·8	—	—	—	—
	*(*a*)	0·0042	0·4938	0·0358	0·0038	0·0005
	**(*b*)	1·730	1·625	—	—	—
1	+(*c*)	1·797	1·645	—	—	—
	++(*d*)	3957·7	4143·1	4345·4	—	—
	*(*a*)	0·0012	0·0033	0·9844	0·0007	0·0221
	**(*b*)	1·788	1·710	1·656	—	—
2	+(*c*)	1·959	1·827	1·690	—	—
	++(*d*)	3814·0	3985·8	4172·1	—	—
	*(*a*)	0·0000	0·0038	0·0017	0·7617	0·0431
	**(*b*)	1·840	1·794	1·735	1·686	—
3	+(*c*)	2·147	1·989	1·861	1·735	—
	++(*d*)	—	—	4016·8	4204·1	4406·9
	*(*a*)	0·0000	0·0002	0·0036	0·3933	—
	**(*b*)	1·890	1·842	1·800	1·745	1·712
4	+(*c*)	2·413	2·180	2·023	1·897	1·780
	++(*d*)	—	—	—	4050·7	4239·1

*(*a*) Morse Franck-Condon factors, **(*b*) *r-centroids* by graphical method in Angstrom, +(*c*) *r-centroids* by quadratic dequation method in Angstroms, ++(*d*) Wavelengths of the observed bands in Angstroms.

SiN was observed by Jevons (1913), Mulliken (1925), Jenkins and De Laszlo (1929), Dunn *et al* (1969). The Franck-Condon factors and r-centroids of this system of SiN has been studied by Stevens and Ferguson (1963) using the Morse potential But recently the study of this band system at high resolution by Bredohl *et al* (1976) has led to new improved molecular parameters for the $B^2\Sigma^+ \rightarrow X^2\Sigma^+$ states of SiN which is an astrophysically important molecule. In view of the above mentioned usefulness of the data and the availability of the improved molecular parameters, the Franck-Condon factors and r-centroids for the B–X band system of SiN have been calculated in this note.

The approximate analytic method of Fraser and Jarmain (1953) applying r_e-shift correction has been used in computing the Franck-Condon factors. The r-centroids have been calculated by quadratic equation method of Nicholls and Jarmain (1956) and these have been verified by graphical method. The values of Franck-Condon factors are found to satisfy the vibrational sum rule. Jarmain *et al* (1956), on basis of the study of a number of band systems, have established that $\Delta r = r_{v'+1,v''+1} - r_{v',v''}$ in a sequence remains constant. This is found to be true in this case also Further, in this case Δr for a sequence is greater than 0·01 Å showing that the two potentials involved in the transition are wide. Also in this case $r_e' - r_e''$ is positive and very small and ω_e' is slightly less than ω_e'', the Condon parabola is narrower which is in complete agreement with the deduced intensity curves by Jevons (1932). The abnormally small values of intensities of many bands are indicative of the fact that the system is perturbed which is in full agreement with the results of Bredohl *et al* (1976).

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References

Bredohl H, Dubois I, Houbrechts Y and Singh M 1976 *Can. J. Phys.* **54** 680
Dunn T M, Rao K M, Nagraj S and Verma R D 1969 *Can. J. Phys.* **47** 2128
Fraser P A and Jarmain W R 1953 *Proc. Phys. Soc.* **A66** 1153
Jarmain W R, Nicholls R W, Perkinson W and Robinson D 1956 *Proc. Phys. Soc.* **A69** 713
Jenkins F A and De Laszlo H 1929 *Proc. Roy. Soc.* **122** 103
Jevons W 1913 *Proc. Roy. Soc.* **A89** 187
Jevons W 1932 *Report on band spectra of diatomic molecules* The Physical Society London
Mulliken R S 1925 *Phys. Rev.* **26** 319
Nicholls R W and Jarmain W R 1956 *Proc. Phys. Soc.* **A69** 253
Stevens A E and Ferguson H L S 1963 *Can. J. Phys.* **41** 240